

Benzenesulfonic acid, 3-hydrazino-
138-30-7 | DTXSID8059681

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 275 °C

Global applicability domain: Inside

Local applicability domain index: 3.44e-01

Confidence level: 4.31e-01

Nearest Neighbors from the Training Set

Image not found

Benzenesulfonic acid, 4-hydrazino-

Measured: 286

Predicted: 279

Image not found

Aminohippuric acid

Measured: 199

Predicted: 201

Image not found

5-Quinolinesulfonic acid, 8-hydroxy-

Measured: 323

Predicted: 197

Image not found

Phthalamide

Measured: 222

Predicted: 208

Image not found

Aspartame

Measured: 247

Predicted: 235